MOLECULAR DYNAMICS SIMULATION OF PINNING OF DISLOCATIONS BY INHOMOGENEOUS PRECIPITATES IN IRON

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Precipitation strengthening in solids (e.g. alloys) is a phenomenon with high technological relevance. Contrary to previous simplifications, knowledge about the chemical inhomogeneity of precipitates grows and hence it is known that e.g."copper precipitates" in steel may be inhomogeneous and can contain additional elements such as Fe, Ni, Mn.

Aiming to understand mechanical properties of alloys from an atomistic point of view, the pinning of dislocations at Cu precipitates has already been demonstrated, see [1]. The present contribution focusses on chemically inhomogeneous precipitates and presents a simulation model to demonstrate the interaction between a moving edge dislocation and such precipitates. The pinning behaviour is shown for homogeneous and inhomogeneous preciptate case. In addition, the way how to derive the increase in strength from the simulation results is shown.

References

[1] S. Nedelcu, P. Kizler, S. Schmauder, and N. Moldovan, “Atomic Scale Modelling of Edge Dislocation Movement in the α-Fe-Cu system,” *Modelling and Simulation in Materials Science and Engineering*, v. 8, p. 181-191, 2000.